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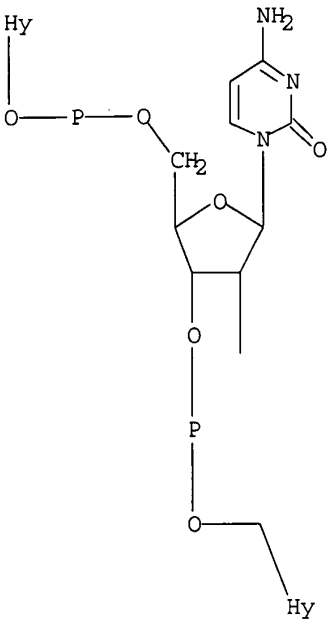

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L3 4 SEA FILE=CAPLUS ABB=ON PLU=ON L2

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L2 14 L1 SSS FULL

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L3 4 L2

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L3 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:127033 CAPLUS
DOCUMENT NUMBER: 136:386341
TITLE: 2'-Ethynyl-DNA: synthesis and pairing properties
AUTHOR(S): Buff, Rolf; Hunziker, Jurg
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Bern, Bern, CH-3012, Switz.
SOURCE: Helvetica Chimica Acta (2002), 85(1), 224-254
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2-Ethynyl-DNA was developed as a potential DNA-selective oligonucleotide analog. The synthesis of 2'-arabino-ethynyl-modified nucleosides was achieved starting from properly protected 2'-ketonucleosides by addition of lithium (trimethylsilyl)acetylide followed by reduction of the tertiary alc. After a series of protecting-group manipulations, phosphoramidite building blocks suitable for solid-phase synthesis were obtained. The synthesis of oligonucleotides from these building blocks was successful when a fast deprotection scheme was used. The pairing properties of 2'-arabino-ethynyl-modified oligonucleotides can be summarized as follows: The 2'-arabino-ethynyl modification of pyrimidine nucleosides leads to a strong destabilization in duplexes with DNA as well as with RNA. The likely reason is that the ethynyl group sterically influences the torsional preferences around the glycosidic bond leading to a conformation not suitable for duplex formation. If the modification is introduced in purine nucleosides, no such influence is observed The pairing properties are not or only slightly changed, and, in some cases (deoxyadenosine homo-polymers), the desired stabilization of the pairing with a DNA complementary strand and destabilization with an RNA complement is observed In oligonucleotides of alternating deoxycytidine-deoxyguanosine sequence, the incorporation of 2'-arabinoethynyl deoxyguanosine surprisingly leads to the formation of a left-handed double helix, irresp. of salt concentration The rationalization for this behavior is that the ethynyl group locks such duplexes in a left-handed conformation through steric blockade.

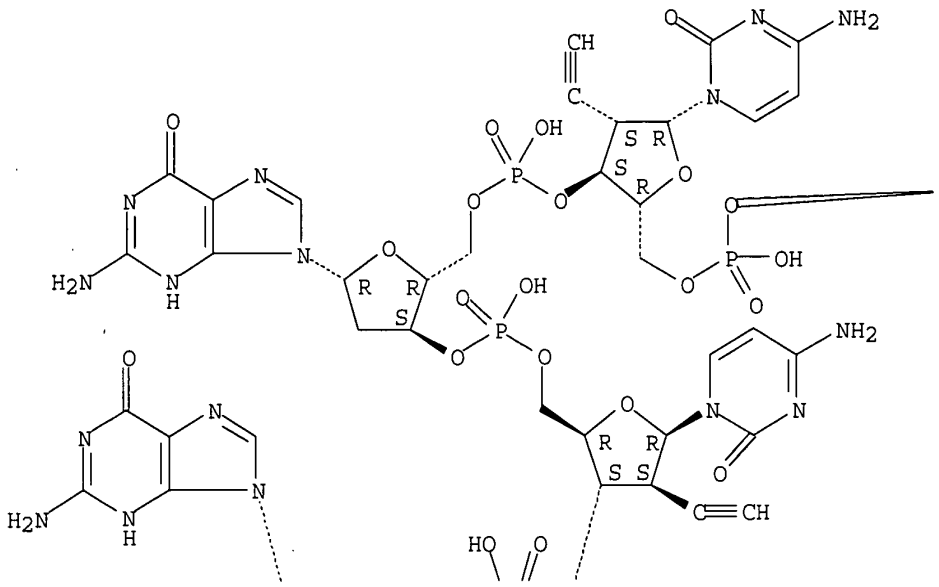
IT **231623-33-9P 424822-71-9P 424822-72-0P**
424822-78-6P 424822-79-7P
RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2'-Ethynyl-DNA to be used in the synthesis and pairing properties of DNA and RNA duplexes)

RN 231623-33-9 CAPLUS

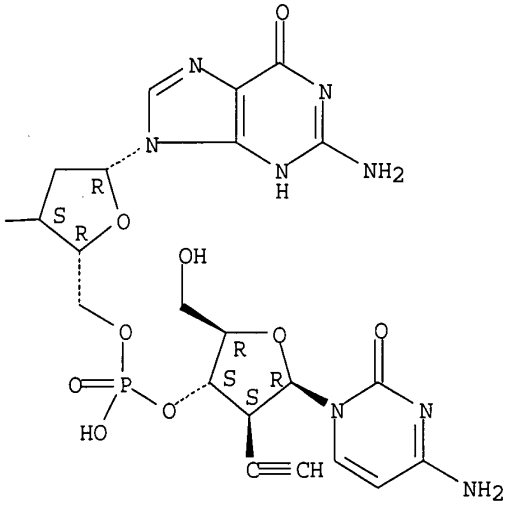
CN Guanosine, 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

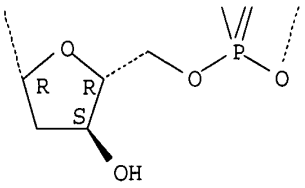
PAGE 1-A



PAGE 1-B



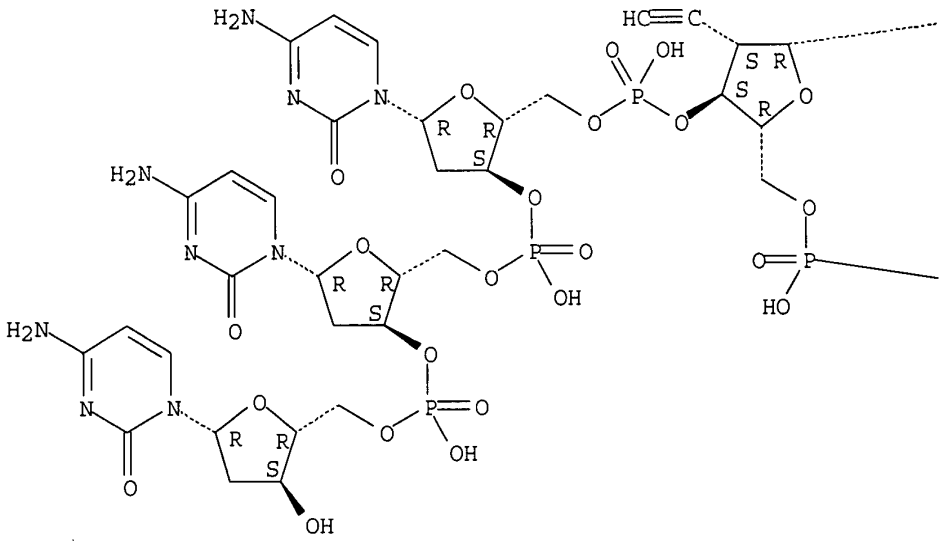
PAGE 2-A



RN 424822-71-9 CAPLUS
CN Cytidine, 2'-deoxycytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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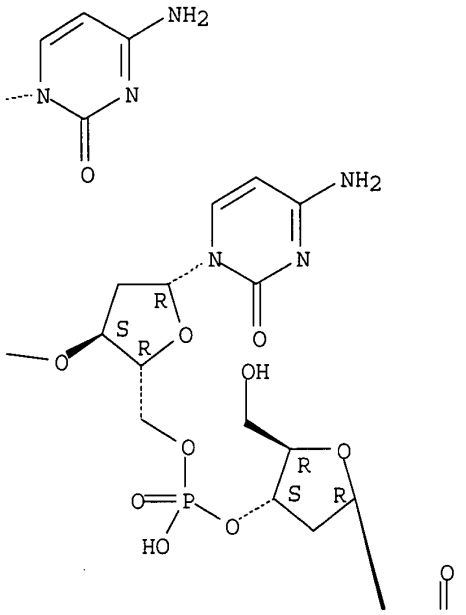

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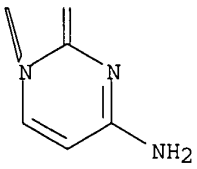
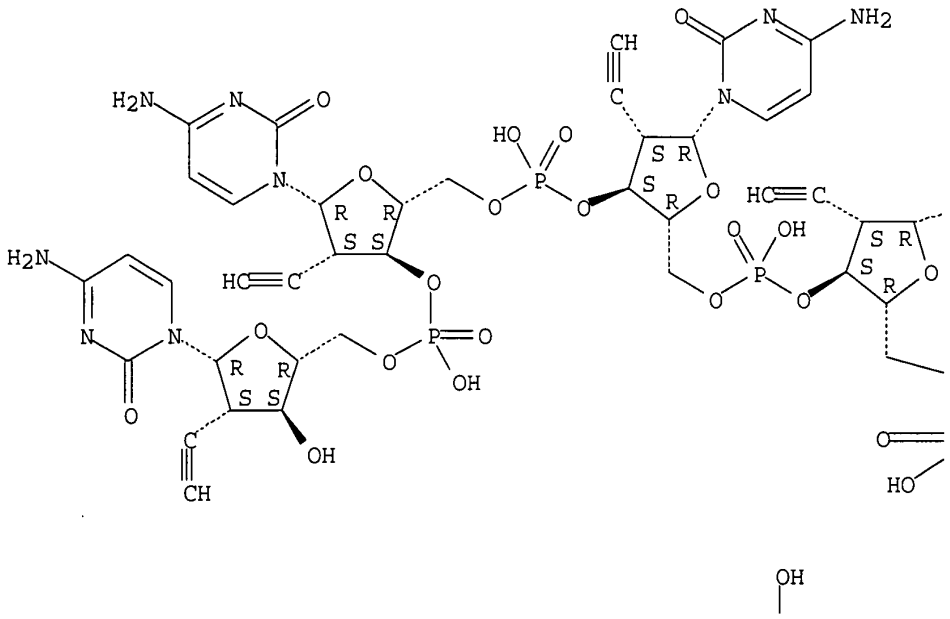


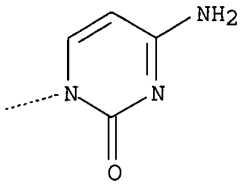
RN 424822-72-0 CAPLUS
CN β-D-arabino-Cytidine, 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-
(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-
(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-
(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-
(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-
(3'→5')-2'-deoxy-2'-ethynyl- (9CI) (CA INDEX NAME)

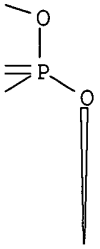
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B





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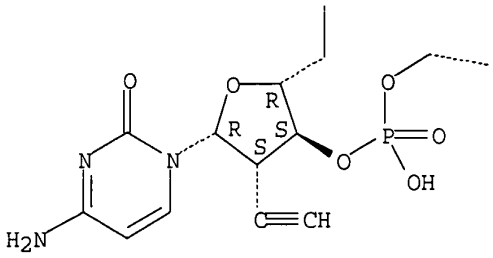

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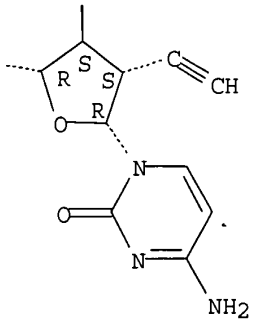
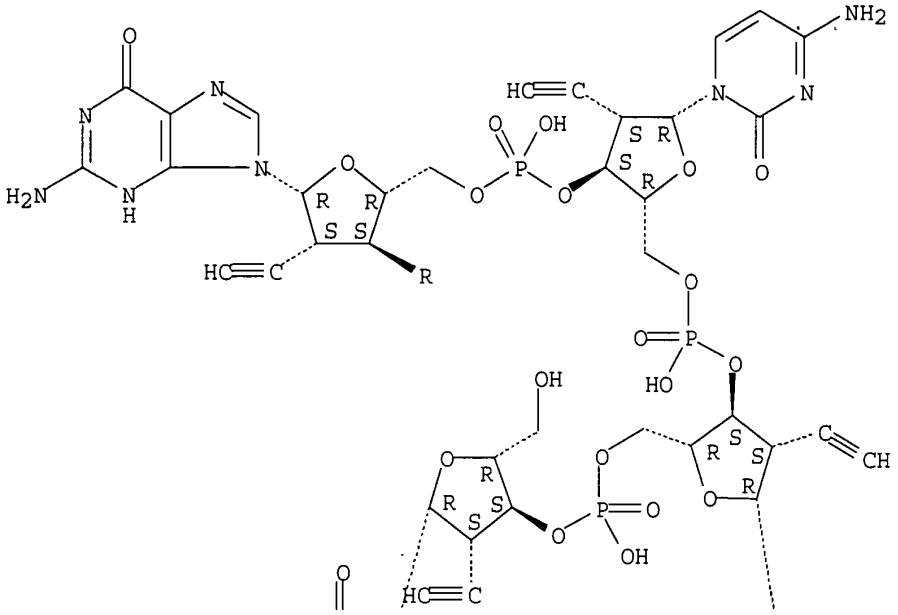


RN 424822-78-6 CAPLUS
CN β-D-arabino-Guanosine, 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-guanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-guanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-2'-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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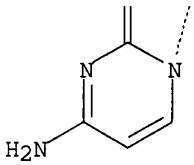
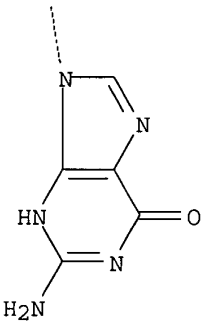
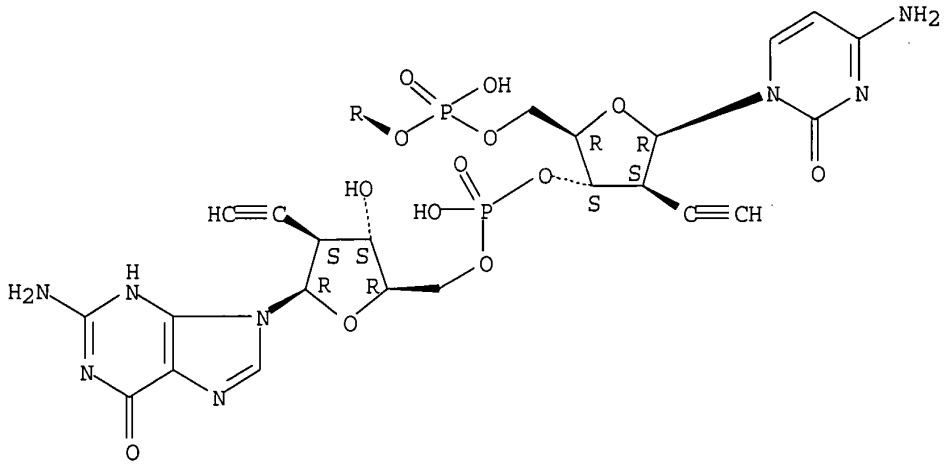




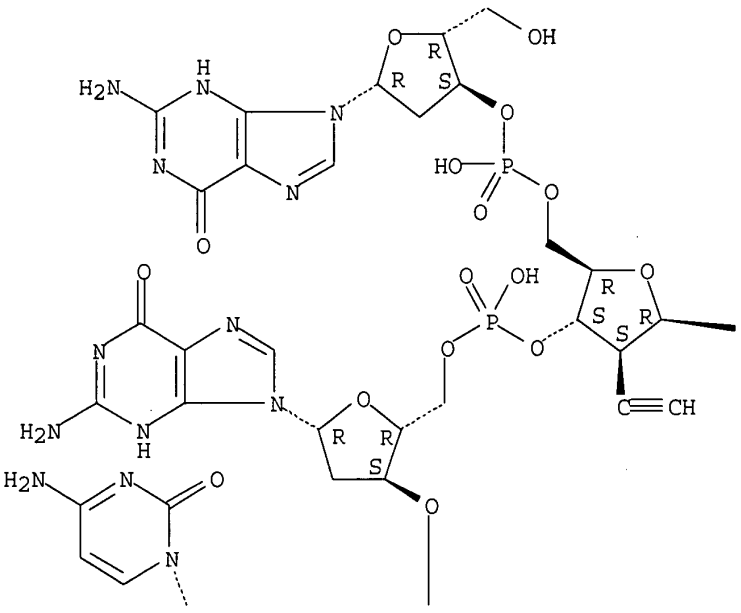
PAGE 3-A



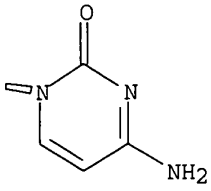
RN 424822-79-7 CAPLUS
CN Cytidine, 2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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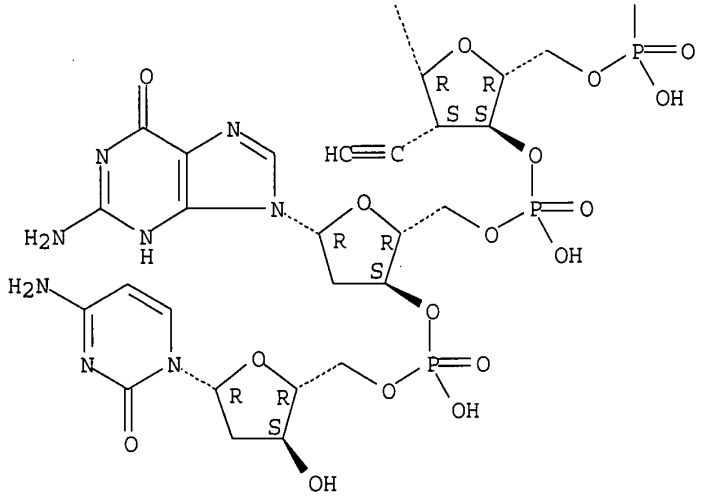


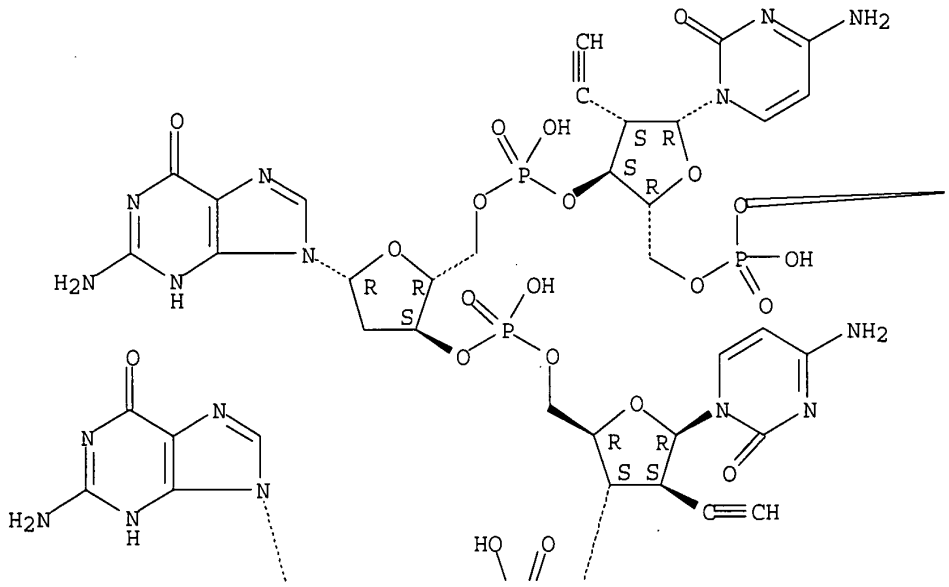
IT **231623-33-9DP**, self-complementary **424822-80-0P**
424822-82-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2'-Ethynyl-DNA to be used in the synthesis and pairing properties of DNA and RNA duplexes)

RN 231623-33-9 CAPLUS

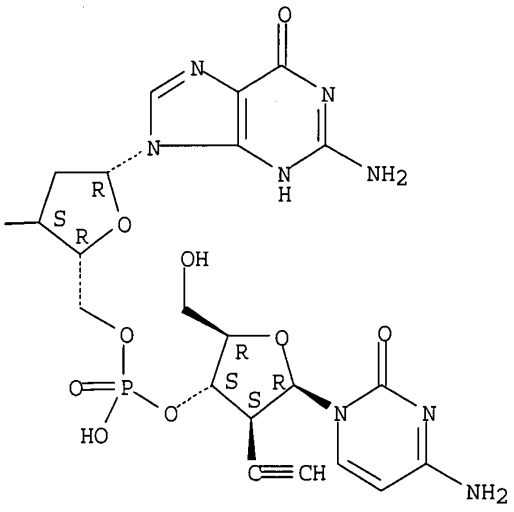
CN Guanosine, 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

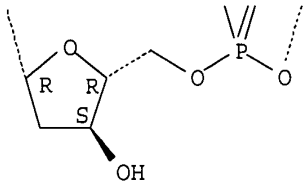
PAGE 1-A



PAGE 1-B



PAGE 2-A



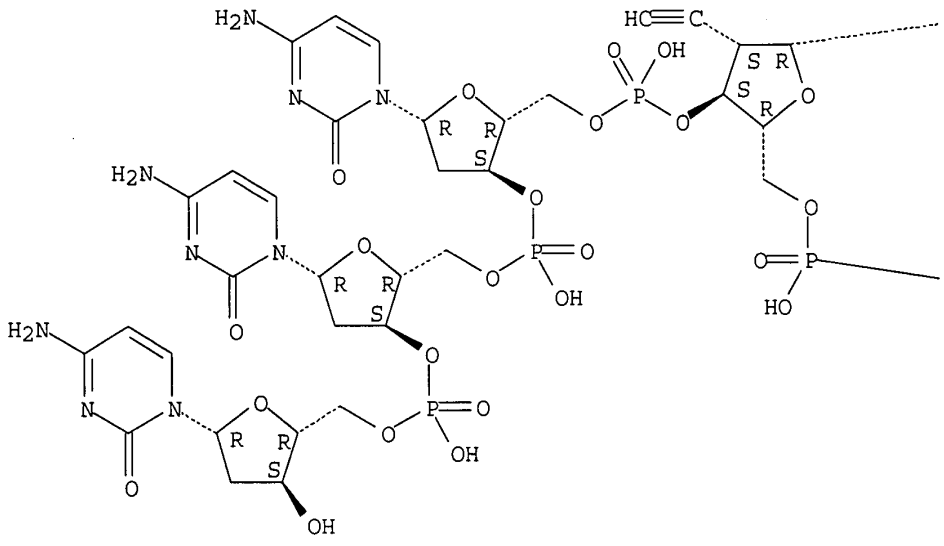
RN 424822-80-0 CAPLUS
CN Guanosine, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with 2'-deoxycytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxycytidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 424822-71-9
CMF C56 H73 N18 O34 P5

Absolute stereochemistry.

PAGE 1-A



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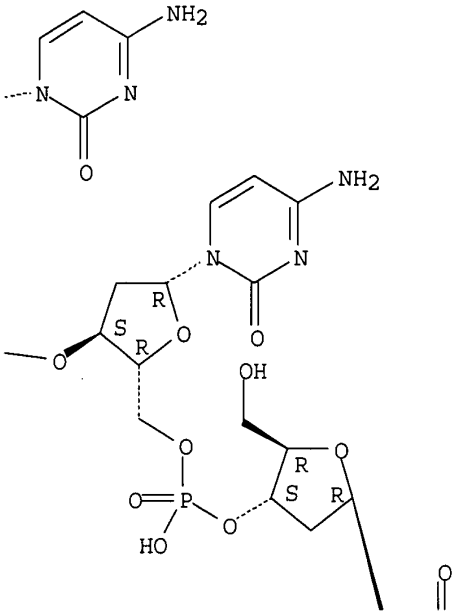

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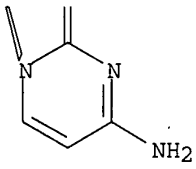
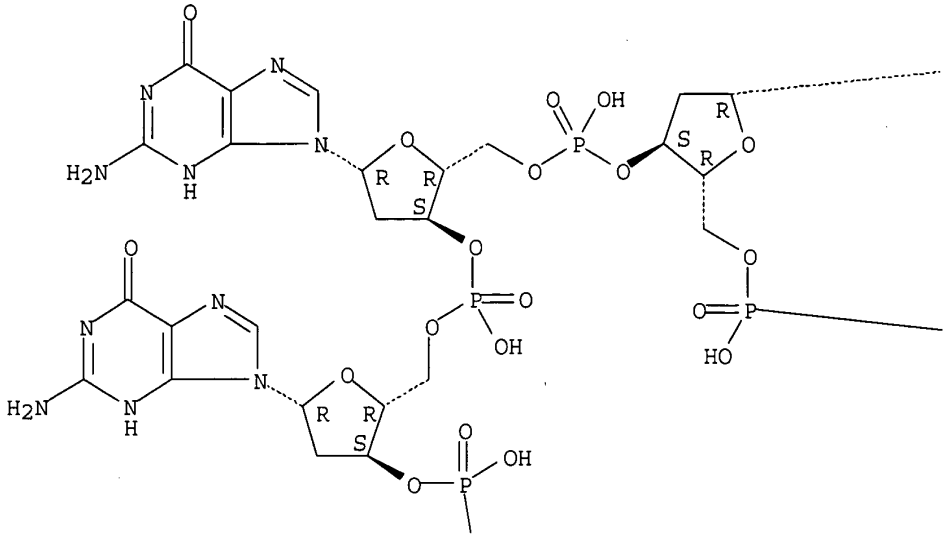


CM 2

CRN 58626-19-0
CMF C60 H73 N30 O34 P5

Absolute stereochemistry.

PAGE 1-A



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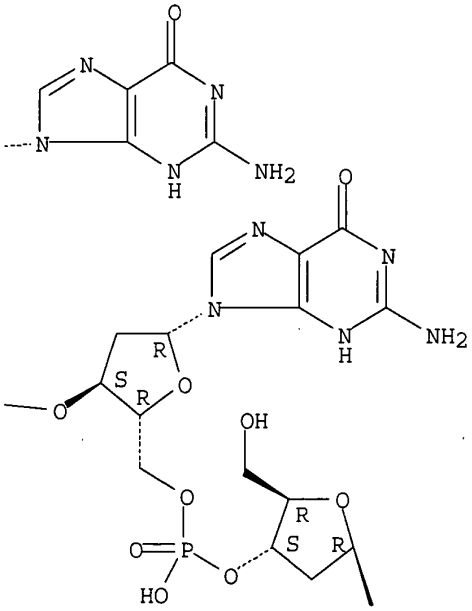

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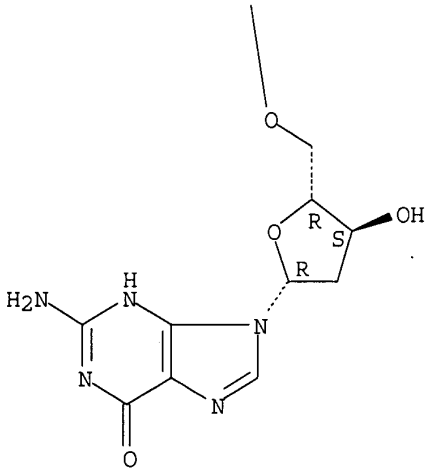
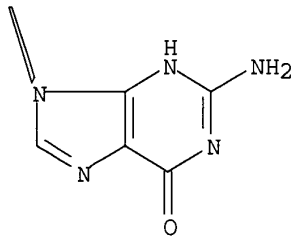


PAGE 2-B



RN 424822-82-2 CAPLUS
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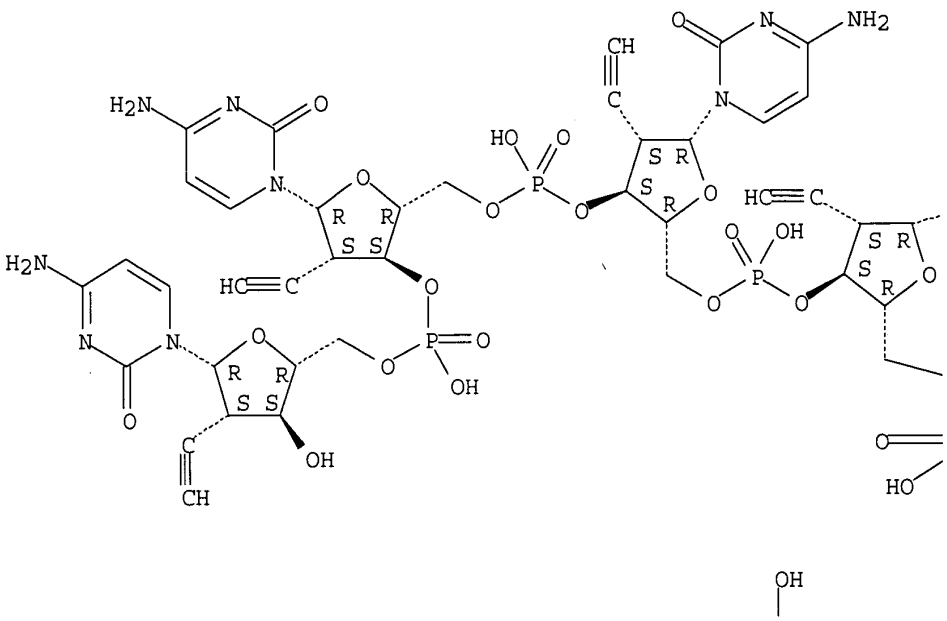
CM 1

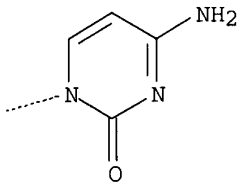
CRN 424822-72-0
CMF C66 H73 N18 O34 P5

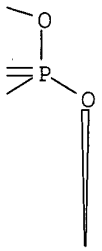
Absolute stereochemistry.

PAGE 1-A

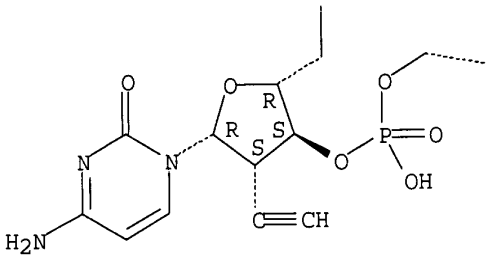


PAGE 1-B





PAGE 2-A



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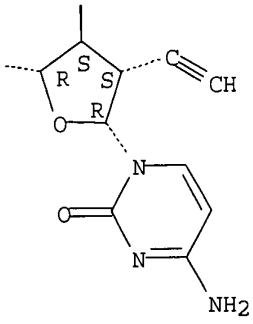
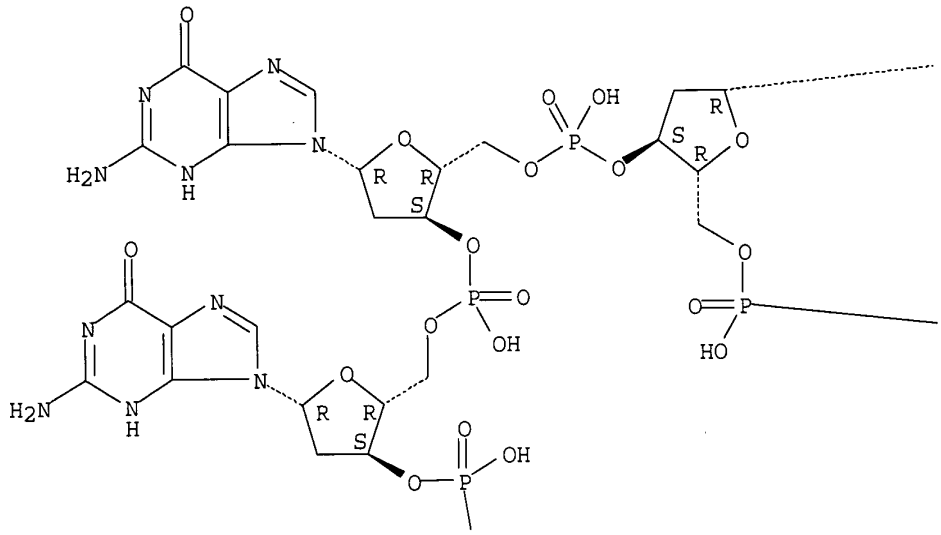


CM 2

CRN 58626-19-0
CMF C60 H73 N30 O34 P5

Absolute stereochemistry.

PAGE 1-A



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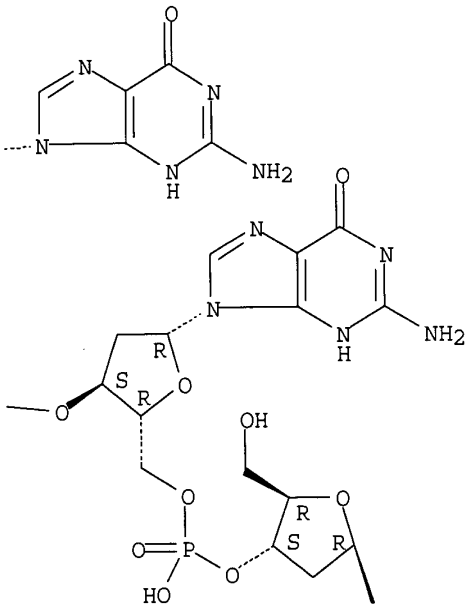

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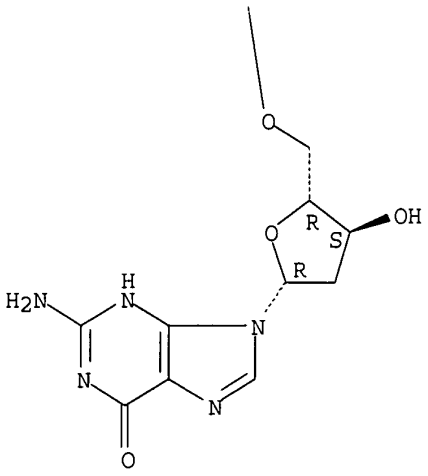

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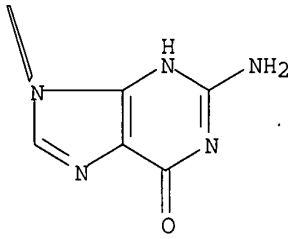


REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:395013 CAPLUS
DOCUMENT NUMBER: 131:102492
TITLE: Z-DNA formation by 2'-C-ethynyl-modified oligonucleotides
AUTHOR(S): Buff, Rolf; Hunziker, Jurg
CORPORATE SOURCE: Department Chemistry Biochemistry, Univ. Bern, Bern, CH-3012, Switz.
SOURCE: Synlett (1999), (Spec.), 905-908
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:102492

AB 9-(2'-Deoxy-2'-C-ethynyl-β-D-arabino-pentofuranosyl)guanine phosphoramidite was prepared from guanosine in 9 steps and incorporated into oligodeoxynucleotides. Substitution of 2 or 3 ethynyl-modified guanosines for deoxyguanosine within d(CG)3 or d(GC)3 leads to a Z-DNA-like conformation of the resulting duplex regardless of salt concentration

IT **231623-33-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)

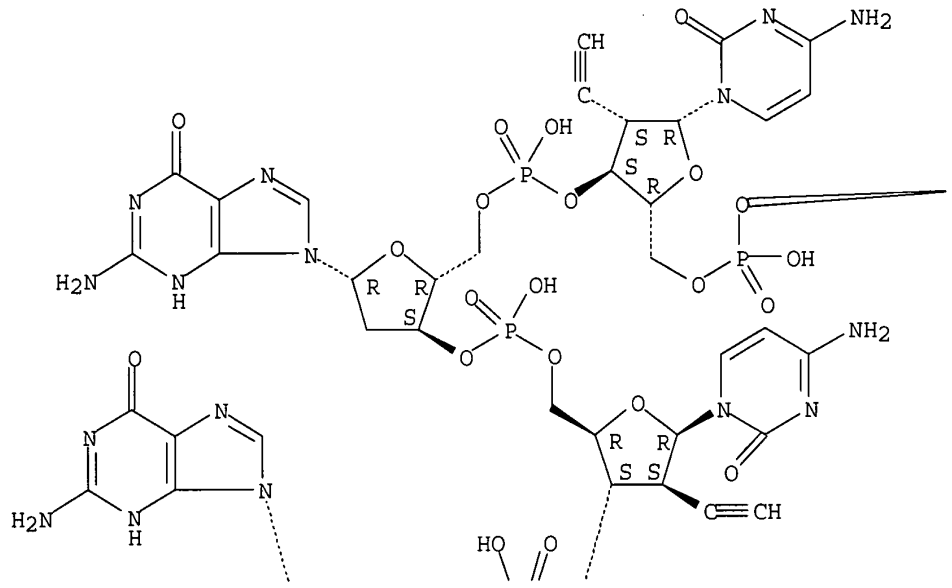
(preparation and Z-DNA formation of ethynyl-guanosine oligonucleotides)

RN 231623-33-9 CAPLUS

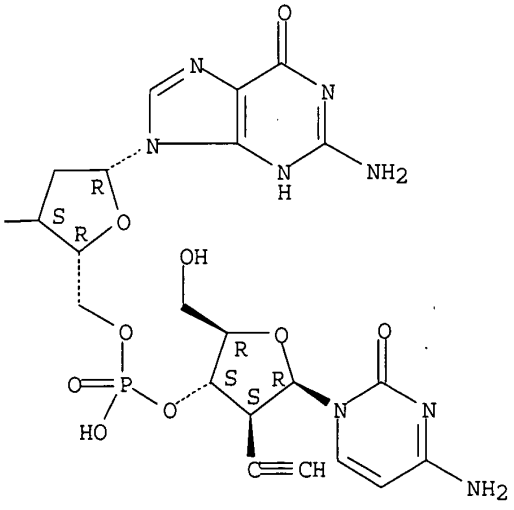
CN Guanosine, 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

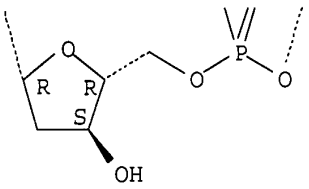
PAGE 1-A



PAGE 1-B



PAGE 2-A



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:17764 CAPLUS
DOCUMENT NUMBER: 130:182710
TITLE: 2'-C-Branched Ribonucleosides: Synthesis of the Phosphoramidite Derivatives of 2'-C-β-Methylcytidine and Their Incorporation into Oligonucleotides
AUTHOR(S): Tang, Xiao-Qing; Liao, Xiangmin; Piccirilli, Joseph A.
CORPORATE SOURCE: Howard Hughes Medical Institute Departments of Biochemistry Molecular Biology and Chemistry, University of Chicago, Chicago, IL, 60637, USA
SOURCE: Journal of Organic Chemistry (1999), 64(3), 747-754
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We describe a strategy for the incorporation of a 2'-C-branched ribonucleoside, 2'-C-β-methylcytidine, into oligonucleotides via solid-phase synthesis using phosphoramidite derivs. 4-N-Benzoyl-2'-C-β-methylcytidine was synthesized by coupling persilylated 4-N-benzoylcytosine with 1,2,3,5-tetra-O-benzoyl-2-C-β-methyl-α-(and β)-D-ribofuranose in the presence of SnCl4 in acetonitrile, followed by selective deprotection with NaOH in pyridine/methanol. The 3'- and 5'-hydroxyl groups were blocked as a cyclic di-tert-butylsilanediyl ether by treatment with di-tert-butyldichlorosilane/AgNO3 in DMF. The 2'-hydroxyl group was then protected as a tert-butyldimethylsilyl ether by treatment with tert-butylmagnesium chloride followed by addition of tert-butyldimethylsilyl trifluoromethanesulfonate in THF. As an alternative to 2'-silyl protection, the corresponding 2'-O-tetrahydropyranyl ether was prepared by treatment with 4,5-dihydro-2H-pyran in the presence of a catalytic amount of 10-camphorsulfonic acid in methylene chloride. The di-tert-butylsilanediyl groups were removed by treatment with pyridinium poly(hydrogen fluoride). Protection of the 5'-hydroxyl group as a dimethoxytrityl ether and phosphitylation of the 3'-hydroxyl group by the standard procedure gave the phosphoramidite derivs. Both these derivs. could be used to incorporate 2'-C-β-methylcytidine into oligonucleotides efficiently via standard solid-phase synthesis, but the tetrahydropyranyl group was more readily removed from oligonucleotides than the tert-butyldimethylsilyl group. Oligonucleotides containing 2'-C-β-methylcytidine undergo base-catalyzed degradation analogous to natural RNA.

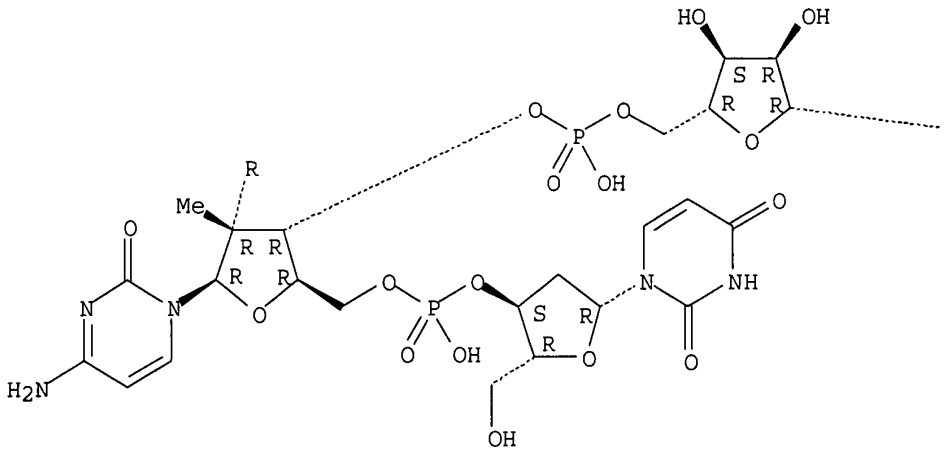
IT **220503-72-0P 220503-75-3P 220503-77-5P**

220503-93-5P 220503-95-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of the phosphoramidite derivs. of 2'-C-β-methylcytidine and their incorporation into oligonucleotides)

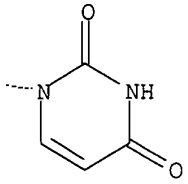
RN 220503-72-0 CAPLUS
CN Uridine, 2'-deoxyuridylyl-(3'→5')-2'-O-[(1,1-dimethylethyl)dimethylsilyl]-2'-C-methylcytidylyl-(3'→5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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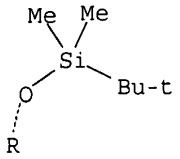
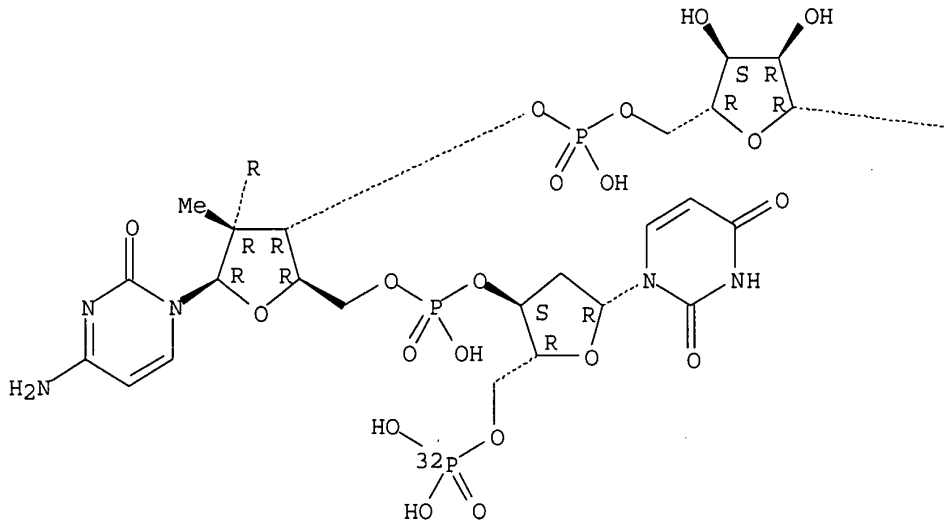


RN 220503-75-3 CAPLUS

CN Uridine, 2'-deoxy-5'-O-(phosphono-32P)uridylyl-(3'→5')-2'-O-[(1,1-dimethylethyl)dimethylsilyl]-2'-C-methylcytidylyl-(3'→5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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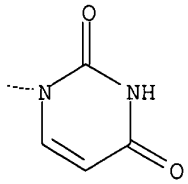
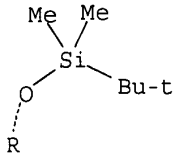
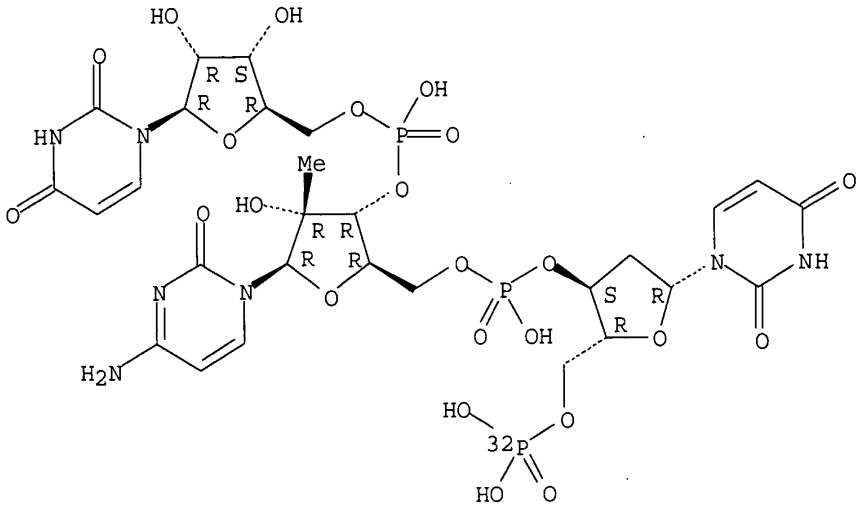


PAGE 2-A



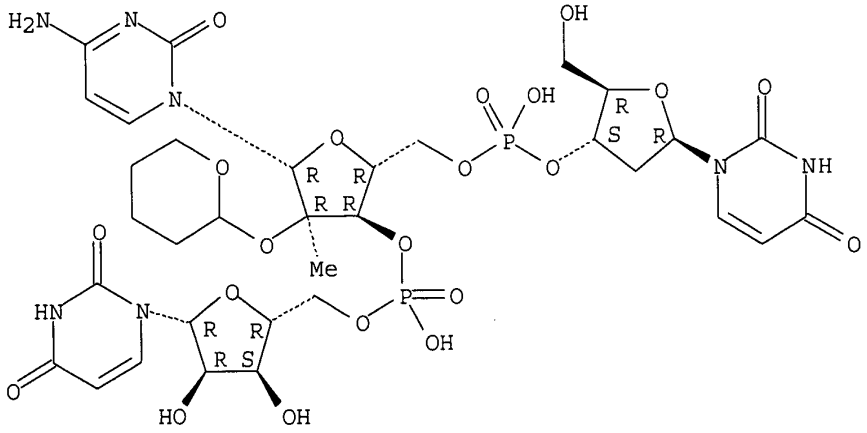
RN 220503-77-5 CAPLUS
CN Uridine, 2'-deoxy-5'-O-(phosphono-32P)uridylyl-(3'→5')-2'-C-methylcytidylyl-(3'→5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



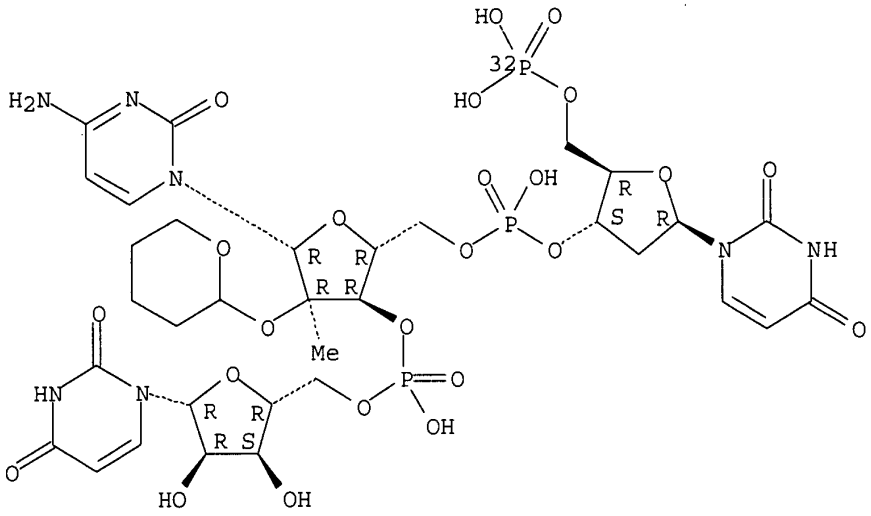
RN 220503-93-5 CAPLUS
CN Uridine, 2'-deoxyuridylyl-(3'→5')-2'-C-methyl-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'→5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 220503-95-7 CAPLUS
CN Uridine, 2'-deoxy-5'-O-(phosphono-32P)uridylyl-(3'→5')-2'-C-methyl-2'-O-(tetrahydro-2H-pyran-2-yl)cytidylyl-(3'→5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:535791 CAPLUS
DOCUMENT NUMBER: 129:276238
TITLE: Preparation of oligonucleotides having 5-fluorouracil moiety
INVENTOR(S): Ozaki, Shoichiro
PATENT ASSIGNEE(S): Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10218893	A2	19980818	JP 1994-308073	19941107

PRIORITY APPLN. INFO.: JP 1994-308073 19941107

AB Oligonucleotides having ≥1 5-fluorouracil moiety, useful as antitumor agents with reduced cytotoxicity, are prepared by binding 5-fluorouridine or 5-fluoro-2'-deoxyuridine 5- or 3-(cyanoethyl phosphoramidite) or 2-(chlorophenyl phosphate) with nucleotides. IC50 of 5-fluorouridylyl-(5'→5')-5-fluorouridine, prepared from 2',3'-O-isopropylidene-5-fluorouridine and β-cyanoethyl phosphorodichloridite with 3 steps, against growth of human gastric cancer cell KATO-III was 0.005 μM, vs. 0.021 μM of 5-fluorouracil.

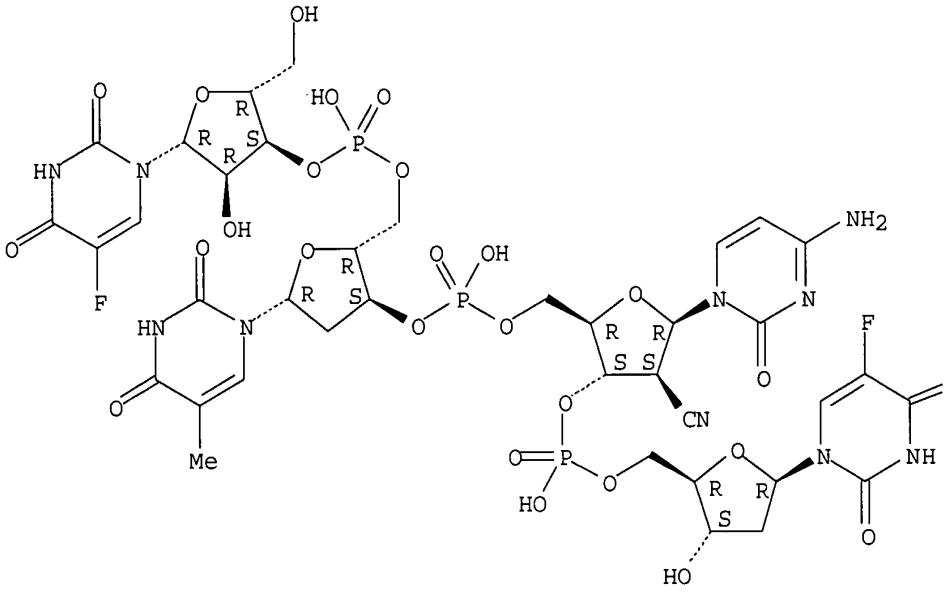
IT **214000-75-6P 214000-76-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oligonucleotides having 5-fluorouracil moiety as antitumor agents)

RN 214000-75-6 CAPLUS

CN Uridine, 5-fluorouridylyl-(3'→5')-thymidylyl-(3'→5')-2'-cyano-2'-deoxy-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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RN 214000-76-7 CAPLUS
CN Uridine, 2'-deoxy-5-fluorouridylyl-(3'→5')-2'-cyano-2'-deoxy-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.